Monica Kosa

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Professional Profile

I am a computational chemist and material scientist with broad experience in molecular and solid state modelling. I published 38 peer-reviewed papers, organized international conferences, serve as a reviewer for scientific journals and funding agencies in US and Europe.

Technical skills

Proficient in modelling packages: CP2K, VASP, Gaussian, Materials Studio, Schroedinger.
Scripting tools: python, perl, bash.

Employment

August 2017-now	PSI-Marie-Skłodowska-Curie Fellow Laboratory for Scientific Computing and Modelling, Paul Scherrer Institut, PSI, Villigen, CH *Modelling extended defects and interfaces of materials with complex electronic structure.*
December 2015-June 2017	Head of the Computational Chemistry Unit Chemistry Faculty, Technion, Haifa, Israel *Various Computational Chemistry projects in the field of Organic Reactivity, in collaboration with experimental groups.* *Budget, computing resources maintenance.*
March 2016-June 2017 *Part time researcher*	Researcher Chemistry Department, Tel Aviv University, Israel *Prof. M. Gozin research group* *Modelling properties of energetic (propellants) molecules and materials.*
2011 - 2015	Researcher, partially as a postdoctoral fellow, Bar-Ilan University (BIU), Ramat Gan, Israel. *Prof. D. T. Major research group* *Modelling of processes occurring in solar cells, Li-ion and Mg-ion batteries, fuel cells.*
2007-2010	Postdoctoral associate, ETH Zurich, Switzerland. *Prof. M. Parrinello research group* *DFT studies of dense hybrid framework materials.*

Education

2001-2007	Ph.D. – Chemistry, Technion. Haifa, Israel, Excellence scholarship. Supervisor: Prof. Y. Apeloig. *Thesis title: Theoretical Studies of Silicon and Metallasilicon Compounds.*
1998-2001	B.Sc. – Chemistry, Technion, Haifa, Israel, *President (twice) and Dean (twice) lists*.

Professional Activities

Research team leadership

October 2016 – June 2017	M.Sc. student project: Computational characterization of iodine rich propellants. Tel Aviv University, Israel
October 2016 – June 2017	M. Sc. student project: Computational characterization and reactivity of metallocorroles. Technion, Israel
2011-2015	2 M.Sc student projects: a) Computational studies of olivine phosphates. b) Electrochemical properties of metallocorroles. Bar Ilan University, Israel
2007-2010	2 Ph.D students, 1 postdoc. ETHZ, Switzerland

International Conference Organization

June 2017	Organizer and initiator of the Lorentz workshop entitled: Fundamental Electrocatalysis: Theory Meets Experiments , Leiden, Netherlands. https://www.lorentzcenter.nl/lc/web/2017/900/info.php3?wsid=900&venue=Oort
September 2016	Organizer and initiator of symposium A06 on "Catalytic Materials and Processes for Energy Storage and Conversion", German Material and Engineering Society, MSE2016, held in Darmstadt, Germany. For the scientific program see: http://www.dgm.de/dgm/mse-congress/#
September 2014	Organizer and initiator of symposium A06 on "Catalytic Materials and Processes for Energy Storage and Conversion", German Material and Engineering Society, MSE2014, held in Darmstadt, Germany. For the scientific program see: http://www.dgm.de/dgm/mse-congress/#
July 2012	Co-organizer of “Users' meeting of the Cyprus International Supercomputing Centre the LinkSceem Project, Bar Ilan University, Ramat Gan, Israel.

Reviewer

Manuscripts submitted to scientific journals, US DOE research proposals - funding, Polish National Science Centre research proposals - funding.

Teaching experience

Organic Chemistry – courses at various levels for students from various departments: chemistry, materials and chemical engineering, biochemistry.
Chemical Kinetics and Surface Chemistry
General (Fundamentals) Chemistry
Analytical chemistry

Workshop Participation

1st German Israeli Battery School, October 2014, Herzlyia, Israel
Mini-DFT course, March 2014, Prof. K. Burke, WIS, Israel
VASP, May 2012, Nantes, France
CP2K, February 2009, Zurich, Switzerland
Gaussian, April 2003, Ulm, Germany
Israeli-German Minerva meeting, September 2002, Blankensee, Germany
Winterschool on Organic reactivity, Winter 2001, Bressanone, Italy

Grants

Grants, awards and non-monetary recognitions

2018-2019	Admitted to PSI, CH, Program for Women with Leadership Ambitions.
2017-2019	PSI-Marie-Skłodowska-Curie, COFUND-personal, CH.
2017	Lorentz centre, NL, workshop organization grant.
2017	PSI-k workshop organization grant.
2011-2013	Ministry of Aliyah and Integration, IL, Returning Scientist Grant, personal.
2001-2007	PhD Excellence scholarship award, Technion, Haifa, IL, personal.
1998-2001	Undergraduate studies, Technion, Haifa, IL, President's list top university student (twice) and Dean's list, top faculty student (twice).

CPU grants, competitive calls

2017-2018	"CSCS", CH
2015-2016	"ARCHER", UK
2016-2017	"Cytera", Cyprus
2012-2013	"Cytera", Cyprus
2010-2011	Madrid Supercomputing Centre, Spain
2008-2009	"Mare Nostrum" Barcelona, Spain

Community Engagement, volunteering activities

2014-2015	Teaching Science in High School, organized by the Trump Foundation, "Schiur be-yahad" section.
2011	Popular Science weekly articles, local city newspaper, in Hebrew.

Languages

English	Fluent
Russian	Fluent
Hebrew	Fluent
German	Basic, A2
Italian	Basic

Communication of Scientific Achievements

List of Publications, Peer Reviewed:

1. Theoretical Study of the Electrocatalytic Reduction of Oxygen by Metallocorroles
   Monica Kosa, Naomi Levy, Lior Elbaz, and Dan Thomas Major
   J. Phys. Chem. C, 2018, *31,*17686-17694.
2. Self-Assembled Cyclic Structures from Copper (II)-Peptoids
   Totan Ghosh, Natalia Fridman, Monica Kosa, Galia Maayan
   Angew.Chem. 2018*, 130,*7829 –7834.
3. Effect of Selective CF_3 Substitution on the Physical and Chemical Properties of Gold Corroles
   K. Sudhakar, A. Mizrahi, M. Kosa, N. Fridman, B. Tumanskii, M. Saphier, Z. Gross
   Angew. Chem. Int. Ed. 2017, 56, 9837.
4. Heteroleptic complexes via solubility control: examples of Cu(II), Co(II), Ni(II) and Mn(II) complexes based on the derivatives of terpyridine and hydroxyquinoline
   Baskin, Maria; Fridman, Natalia; Kosa, Monica; Maayan, Galia
   Dalton Trans., 2017*,*46, 15330-15339
5. The effect of water on the stability of quaternary ammonium groups for anion exchange membrane fuel cell applications
   Dekel, Dario; Amar, Michal; Willdorf, Sapir; Kosa, Monica; Dhara, Shubhendu; Diesendruck, Charles
   Chem. Mater., 2017, 29 (10), pp 4425–4431
6. Energetic, Insensitive and Thermostable Isomers of 1,2,4,5-Tetrazine-bis-1,2,4-Triazoles with Low Toxicity.
   A. Shlomovich, T. Pechersky, A. Cohen, Q. L. Yan, M. Kosa, N. Petrutik, A. Aizikovich and M. Gozin
   Dalton Trans., 2017, 46, 5994.
7. The Planar Cyclooctatetraene Bridge in Bis-Metallic Macrocycles: Isolating or Conjugating?
   Susovan Bhowmik, Monica Kosa, Amir Mizrahi, Natalia Fridman, Magal Saphier, Amnon Stanger and Zeev Gross.
   Inorg. Chem., 2017, 56 (4), pp 2287–2296.
8. Unique Behavior of Dimethoxyethane (DME)/$Mg(N(SO_2CF_3)_2)_2$ Solutions
   Michael Salama, Ivgeni Shterenberg, Haim Gizbar, Neta Nitoker Eliaz, Monica Kosa, Keren Keinan-Adamsky, Michal Afri, Linda J.W. Shimon, Hugo E. Gottlieb, Dan Thomas Major, Yosef Gofer, and Doron Aurbach
   J. Phys. Chem. C, 2016, 120 (35), pp 19586–19594.
9. A Combined Computational and Experimental Investigation of Mg Doped α-Fe_2O_3.
   Monica Kosa, Hannah Noa Barad, Vijay Singh, David A. Keller, Klimentiy Shimanovich, Sven Rühle, Assaf Y. Anderson, Arie Zaban, Dan T. Major.
   Physical Chemistry Chemical Physics, 2016, *18*, 781 - 791
10. Electrochemical and Kinetic Studies of LiNi0.5Co0.2Mn0.3O2 as a Positive Electrode Material for Li-ion Batteries using First Principles
    Mudit Dixit, Monica Kosa, Onit Srur Lavy, Boris Markovsky, Doron Aurbach, and Dan Thomas Major
    Phys. Chem. Chem. Phys., 2016, 18, 6799-6812
11. First-principles evaluation of the inherent stabilities of pure LixMPO4 (M=Mn, Fe, Co,) and Mixed Binary LixFeyM'1-yPO4 (M'=Mn, Co) Olivine Phosphates
    Monica Kosa, Doron Aurbach and Dan Thomas Major
    Materials Chemistry and Physics, Volume 174, 1 May 2016, Pages 54–58
12. Is it True that the Normal Valence-Length Correlation is Irrelevant for Metal-Metal Bonds? Vijay Singh, Mudit Dixit, Monica Kosa, Dan T. Major, Elena Levi, Doron Aurbach. 2016, *Chemistry, a European Journal*, Volume 22, Issue 15, April 4, 2016, Pages 5269–5276

13. Magnetism in Olivine-type $LiCo_{1-x}Fe_xPO_4$ Cathode Materials: Bridging Theory and Experiment. Vijay Singh, Elena Gershinsky, Monica Kosa, Mudit Dixit, David Zitoun, Dan T. Major. *Physical Chemistry Chemical Physics*, 2015, *17*, 31202 – 31215
14. Metallocorroles as Nonprecious-Metal Catalysts for Oxygen Reduction.
    Naomi Levy, Atif Mahammed, Monica Kosa, Dan T. Major, Zeev Gross, Lior Elbaz.
    Angew. Chem. Intl. Ed., 2015, *127*, 14286–14290
15. Electrochemical Interfaces for Energy Storage and Conversion.
    Clotilde S. Cucinotta and Monica Kosa.
    Encyclopedia of Nanotechnology, Springer Science, 2015.
    DOI 10.1007/978-94-007-6178-0_100941-1
16. Classical and Quantum Modeling of Li and Na Diffusion in $FePO_4$
    Mudit Dixit, Hamutal Engel, Reuven Eitan, Doron Aurbach, Michael D. Levi, Monica Kosa, Dan T. Major.
    J. Phys. Chem. C., 2015, *119*, 15801–15809.
17. Structural trends in hybrid perovskites $Me_2NH_2MHCOO_3$ (M = Mn, Fe, Co, Ni, Zn): computational assessment based on Bader charge analysis. ***Invited Paper***
    Monica Kosa, Dan T. Major.
    CrystEngComm. 2015, 17, 295-298.
18. Studies of Aluminum-Doped $LiNi_{0.5}Co_{0.2}Mn_{0.3}O_2$: Electrochemical Behavior, Aging, Structural Transformations, and Thermal Characteristics.
    Aurbach D, Srur-Lavi O, Ghanty C, Dixit M, Haik O, Talianker M, et al.
    Journal of the Electrochemical Society, 2015,162, A1014-A27.
19. Putting DFT to the Test: A First-Principles Study of Electronic, Magnetic, and Optical Properties of Co_3O_4.
    Vijay Singh, Monica Kosa, Koushik Majhi, Dan T. Major.
    Journal of Chemical Theory and Computation. 2015, *11*, 64-72.
20. Topotactic elimination of water across a C-C ligand bond in a dense 3-D metal-organic framework.
    Hamish H.-M. Yeung, Monica Kosa, John M. Griffin, Clare P. Grey, Dan T. Major, Anthony K. Cheetham.
    Chemical Communications, 2014, *50*, 13292-5.
21. Were Reactions of Triplet Silylenes Observed?
    Monica Kosa, Miriam Karni and Yitzhak Apeloig
    J. Am. Chem. Soc., 2013, *135*, 9032-9040.
22. Controlling Dye Aggregation, Injection Energetics and Catalytic Recombination in Organic Sensitizer Based Dye Cells using a Single Electrolyte Additive.
    Sophia Buhbut, John Noel Clifford, Monica Kosa, Asaf Anderson, Menny Shalom, Dan T. Major, Emilio Palomares and Arie Zaban.
    Energy Environ. Sci., 2013, *6,* 3046-3053.
23. A Systematic First-Principles Investigation of Mixed Transition Metal Olivine Phosphates $LiM_{1-y}M'_yPO_4$ (M/M'=Mn, Fe, Co) As Cathode Materials
    Alina Osnis‡, Monica Kosa‡, Doron Aurbach and Dan T. Major. ‡ equally contributing author.
    J. Phys.Chem. C, 2013*, 117*, 17919–17926.
24. Lithium Tartrate Framework Polymorphs: A Detailed Structural Analysis.
    Hamish Yeung, Monica Kosa, Michele Parrinello, Anthony Cheetham.
    Crystal Growth and Design, 2013, *13,* 3705.
25. Negative Linear Compressibility of a Metal-Organic Framework.
    W. Li, M. R. Probert, M. Kosa, T. D. Bennett, A. Thirumuragan, R. P. Burwood, M. Parrinello, J. A. K. Howard, A. K. Cheetham
    J. Am. Chem. Soc., 2012*, 134*, 11940–11943.
26. Ab initio Molecular Dynamics study of the dehydroxylation reaction in a smectite model.
    D. Muñoz-Santiburcio, M. Kosa, A. Hernández-Laguna, C.I. Sainz-Díaz and M. Parrinello.
    J. Phys. Chem. C, 2012, *116*, 12203.

27. Structural diversity and energetics in anhydrous lithium tartrates: experimental and computational studies of novel chiral polymorphs and their racemic and meso analogues. Hamish H.-M. Yeung, Monica Kosa, Michele Parrinello, Paul M. Forster, Anthony K. Cheetham. *Crystal Growth and Design*, 2011, *11*, 221.
28. Probing the Mechanical Properties of Hybrid Inorganic-Organic Frameworks: A Computational and Experimental study.
    Monica Kosa, Jin-Chong Tan, Crystal A. Merrill, Matthias Krack, Anthony K. Cheetham, Michele Parrinello.
    ChemPhysChem, 2010, *11*, 2332. ***FRONT COVER***.
29. Phase Selection and Energetics in Chiral Alkaline-Earth Tartrates and their Racemic and Meso Analogues; Synthetic, Structural, Computational and Calorimetric Studies.
    Leah N. Appelhans, Monica Kosa, Radha Venkataramana, Petra Simoncic, Alexandra Navrotsky, Michele Parrinello, Anthony K. Cheetham.
    J. Am. Chem. Soc., 2009*, 131,* 15375.
30. Bifunctional Catalysis by Natural Cinchona Alkaloids: A Mechanism Explained.
    Clotilde S. Cucinotta, Monica Kosa, Paolo Melchiorre, Andrea Cavalli, Francesco L. Gervasio.
    Chemistry, a Eurpean Journal, 2009, *15,* 7913.
31. Modeling the Hydrogen Storage Materials with Exposed M^{2+} Coordination Sites.
    Monica Kosa, Matthias Krack, Anthony K. Cheetham, Michele Parrinello.
    Journal of Physical Chemistry C, 2008, *112,* 16171.
32. A Theoretical Study of Ladder Polysilanes.
    Monica Kosa, Miriam Karni, Yitzhak Apeloig.
    Organometallics, 2007, *26*, 2806 –2814.
33. Trisilaallene and the Relative Stability of Si_3H_4 Isomers. A Theoretical Study.
    Monica Kosa, Miriam Karni, Yitzhak Apeloig.
    Journal of Chemical Theory and Computation, 2006, *2*, 956-964.
34. Mercury-Substituted Silyl Radical Intermediates in Formation and Fragmentation of Geminal Dimercury Silyl Compounds. Dmitry Bravo-Zhivotovskii, Ilya Ruderfer, Michael Yuzefovich, Monica Kosa, Mark Botoshansky, Boris Tumanskii and Yitzhak Apeloig.
    Organometallics, 2005, *24*, 2698-2704.
35. Kinetic stabilization of polysilyl radicals. Kravchenko V., Bravo-Zhivotovskii D., Tumanskii B., Botoshansky M., Sigal N., Molev G., Kosa M. and Apeloig Y.
    Organosilicon Chemistry VI ", N. Auner and J. Weis, Editors, VCH, (2005).
36. How to design linear allenic trisilaallenes and trigermaallenes.
    Monica Kosa, Miriam Karni and Yitzhak Apeloig.
    J. Am. Chem. Soc., 2004, *126*, 10544-10545.
37. The direct synthesis of a silene-organometallic complex.
    D. Bravo-Zhivotovskii, H. Peleg-Vasserman, M. Kosa, G. Molev, M. Botoshanskii, Y. Apeloig.
    Angew. Chem., Int. Ed. 2004, *43*, 745-748.
38. Relative Stabilities of Spirocyclopropanated Cyclopropyl Cations.
    S. I. Kozhushkov, T. Spath, M. Kosa, Y. Apeloig, D. S.Yufit, and A. de Meijere.
    Eur. J. Org. Chem. 2003, 4234-4242.

Public Oral Presentations

1. E-MRS 2018 Spring meeting, Strasbourg, France, June 2018. Title: “DFT+U gamma-surfaces of UO_2”.
2. LSM, Laboratory for Simulation and Modelling Seminar, PSI, CH, June 2018. Title: “Atomistic simulations of UO_2 – towards extended defects modelling in oxides”.

3. *Materials: Past Present and Future*. Conference to honor Prof. Tony Cheetham's 70th birthday. Madingley Hall, Cambridge University, UK, June 2016, ***Invited Talk***. Title: "Metallocorroles as Nonprecious-Metal Catalysts for Oxygen Reduction. A Computational Perspective".
4. Chemistry Faculty, Technion, Haifa, Israel, April 2016. Title: "Chemistry and Materials of Energy Storage and Generation Devices. A Computational Perspective."
5. Israeli Material Engineering Conference, IMEC, Bar Ilan University, Ramat Gan, Israel, February 2016. Title: "First Principles Investigation of Metallocorroles as Non-Precious Metal Catalysts for Oxygen Reduction Reaction".
6. Department of Engineering, Oxford University, UK, May 2015, ***Invited talk***. Title: "Modelling Materials for Energy Conversion Systems".
7. Israeli-German Battery School, October 2014: Title: "Unraveling the Complex Properties of Transition Metal Olivine Phosphates as Cathode Materials. A Computational Perspective"
8. Israeli Material Engineering Conference, IMEC, Techion, Haifa, Israel, February 2014. Title: "Designing Energy Efficient Materials *in Silico*: the case of Fe_2O_3. A computational and experimental study".
9. Solar fuels conference, Israel, Zichron Yakov, Israel, October 2013. Title: "Designing Energy Efficient Materials *in Silico*: the case of Fe_2O_3".
10. European Congress on Advanced Materials and Processes, EUROMAT, Seville, Spain, September 2013. Oral presentation and a session chair, *Symposium* B4I. Title: "Modeling Dense Hybrid Framework Materials"
    European Congress on Advanced Materials and Processes, EUROMAT, Seville, Spain, September 2013. Oral presentation, *Symposium* D3IV. Title: "Unraveling the Complex Properties of Transition Metal Olivine Phosphates as Cathode Materials. A Computational Perspective."
11. Israelectrochemistry Conference, Bar-Ilan University, Ramat Gan, Israel, June 2013. Title: "Unraveling the Complex Properties of Transition Metal Olivine Phosphates as Cathode Materials. A Computational Perspective".
12. Faculty of Natural Sciences, Department of Biological Chemistry, Ariel University, Israel, April 2013, ***Invited Seminar***. Title: " Discovering Material Properties: A Computational Perspective".
13. Faculty of Sciences, University of Geneva, Geneva, Switzerland, 2012, ***Invited Seminar***. Title: "Discovering Material Properties: A Computational Perspective on Energy Viable Systems."
14. Israeli Material Engineering Conference, IMEC, Dead Sea, Israel 2012.
15. European Congress on Advanced Materials and Processes, EUROMAT, Montpellier, France 2011.
16. European Material Research Society Spring Meeting, EMRS, Strasbourg, France, 2010, ***Best Oral Presentation Award***.
17. High Performance Computing Meeting, Madrid, Spain, 2009
18. Department of Materials Science & Metallurgy, Cambridge, UK, 2009
19. Department of Chemistry and Applied Biosciences - ETH Zurich, Lugano, Switzerland 2009
20. Department of Chemistry and Applied Biosciences - ETH Zurich, Lugano, Switzerland 2008
21. Department of Chemistry and Applied Biosciences - ETH Zurich, Lugano, Switzerland 2007
22. Chemistry Department Seminar, Technion, Haifa Israel 2006
23. Chemistry Department Seminar, Technion, Haifa Israel 2006
24. Lise Meitner-Minerva Symposium, Jerusalem Israel, 2005